Tris(2-hydroxyethyl) isocyanurate

839-90-7 | DTXSID4026266

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.66e-01

Global applicability domain: Outside

Local applicability domain index: 3.28e-01

Confidence level: 7.20e-01

Nearest Neighbors from the Training Set

Image not found

3,7-Dimethyluric acid
Measured: -1.33
Predicted: -1.03

Image not found

1,3-Dimethyluric acid
Measured: -0.520
Predicted: -0.569